Thermal noise can facilitate energy transformation in the presence of entropic barriers

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Abstract

Efficiency of a Brownian particle moving along the axis of a three-dimensional asymmetric periodic channel is investigated in the presence of a symmetric unbiased force and a load. Reduction of the spatial dimensionality from two or three physical dimensions to an effective one-dimensional system entails the appearance of entropic barriers and an effective diffusion coefficient. The energetics in the presence of entropic barriers exhibits peculiar behavior which is different from that occurring through energy barriers. We found that even on the quasistatic limit there is a regime where the efficiency can be a peaked function of temperature, which indicates that thermal noise can facilitate energy transformation, contrary to the case of energy barriers. The appearance of entropic barriers may induce optimized efficiency at a finite temperature.

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INTRODUCTION

Noise-induced transport play a crucial role in many processes from physical and biological to social systems. There has been an increasing interest in transport properties of nonlinear systems which can extract usable work from unbiased nonequilibrium fluctuations [1, 2, 3, 4]. This comes from the desire of understanding molecular motors [5], nanoscale friction [6], surface smoothening [7], coupled Josephson junctions [8], optical ratchets and directed motion of laser cooled atoms [9], and mass separation and trapping schemes at microscale [10].

Most studies have referred to the consideration of the energy barriers. The nature of the energy barriers depends on which thermodynamic potential varies when passing from one well to the other, and its presence plays an important role in the dynamics of the solid-state physics system. However, in some cases, such as soft condensed-matter and biological systems, the entropic barriers should be considered. The entropic barriers may appear when coarsening the description of a complex system for simplifying its dynamics. Reguera and co-workers [11, 12] used the mesoscopic nonequilibrium thermodynamics theory to derive the general kinetic equation of a system and analyze in detail the case of diffusion in a domain of irregular geometry in which the presence of the boundaries induces entropic barriers when approaching the dynamics by a coarsening of the description. In the presence of entropic barriers, the asymmetry of the tube can induce a net current in the absence of any net macroscopic forces or in the presence of the unbiased forces [13].

In recent years the energetics of these systems, which rectify the zero-mean fluctuations, was investigated. Much of the interest was motivated by the elegant piece of work done by Magnasco [14], which showed that a Brownian particle, subject to external fluctuations, can undergo a non-zero drift while moving under the influence of an asymmetric potential. He claimed that there is a region where the efficiency can be optimized at a finite temperature and the existence of thermal fluctuations facilitate the efficiency of energy transformation. His claim is interesting because thermal noise is usually known to disturb the operation of machines. Based on energetic analysis of the same model Kamegawa and co-workers [15] made a important conclusion that the efficiency of energy transformation on the quasistatic limit cannot be optimized at finite temperatures and that the thermal fluctuations does not facilitate it. Takagi and Hondou[16] found that thermal noise may facilitate the energy

conversion in the forced thermal ratchet when an "oscillating ratchet" was considered. A recent investigation of Dan and co-workers [17] showed that the efficiency can be optimized at a finite temperature in inhomogeneous systems with spatially varying friction coefficient in a forced thermal ratchet. Sumithra and co-workers [18] studied a homogeneous ratchet driven by a nonadiabatical external periodic force and found that thermal noise can facilitate the energy transformation. When an isothermal ratchet driven by a chemical reaction between the two states, the efficiency can also have a maximum as a function of temperature [19]. In forced undamped ratchets [20], the efficiency optimization can also be found. In two-dimensional ratchet, Wang and Bao [21] found that the efficiency is peaked function of temperature which is different from that in one-dimensional ratchet. Recently, Ghosh and co-workers [22] investigated the stochastic energetics of direction quantum transport due to rectification of nonequilibrium thermal fluctuations and found that the Stokes efficiency reaches a maximum at a particular temperature. Efficiency optimization in forced thermal ratchet usually takes place for fast oscillating or fluctuation forces. When the force changes very slowly enough, for example a square wave with a very long period, the system can be treated as quasistatic. When the unbiased force is asymmetry, Ai and co-workers [4] found that the thermal noise can facilitate the energy transformation even on the quasi-static limit.

The previous works on efficiency were on the consideration of the energy barriers. The present work is extended to the study of efficiency to the case of entropic barriers. We emphasize on finding whether the thermal noise in the presence of entropic barriers can facilitate the energy transformation even on the quasistatic limit.

EFFICIENCY IN A THREE-DIMENSIONAL PERIODIC TUBE

We consider an overdamped Brownian particle moving in an asymmetric periodic tube [Fig. 1(a)] in the presence of a symmetric unbiased external force and a load. Its overdamped dynamics is described by the following Langevin equations[11, 12, 13]

$$\gamma \frac{dx}{dt} = F(t) - f + \xi_x(t), \tag{1}$$

$$\gamma \frac{dy}{dt} = \xi_y(t), \tag{2}$$

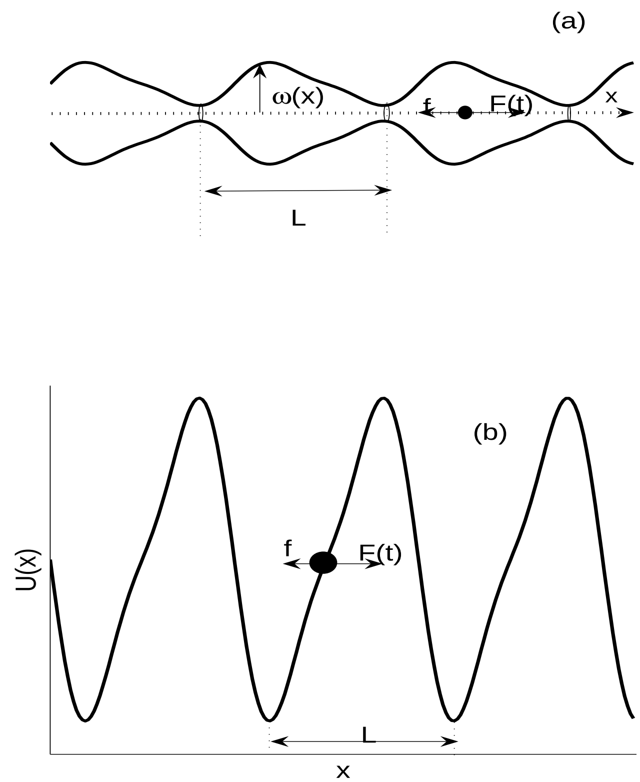

FIG. 1: Schematic diagrams of a tube and a conventional energetic ratchet. (a) A tube with periodicity L. The half-width $\omega(x)$ is a periodic function of x, $\omega(x) = a[\sin(\frac{2\pi x}{L}) + \frac{\Delta}{4}\sin(\frac{4\pi x}{L})] + b$. Δ is the asymmetric parameter of the tube shape. $F(t)$ and f are the zero-mean periodic force and the external load, respectively. (b)The conventional energetic ratchet with periodicity L. $U(x) = -U_0[\sin(\frac{2\pi x}{L}) + \frac{\Delta}{4}\sin(\frac{4\pi x}{L})]$. U_0 is amplitude of the potential and Δ the asymmetric parameter of the potential. $F(t)$ and f are the same as that in (a).

$$\gamma\frac{dz}{dt} = \xi_z(t), \tag{3}$$

where x, y, z are the three-dimensional (3D) coordinates, γ is the friction coefficient of the particle. $\xi_{x,y,z}(t)$ are the uncorrelated Gaussian white noises with zero mean and correlation function: $<\xi_i(t)\xi_j(t') >= 2\gamma k_B T\delta_{i,j}\delta(t-t')$ for $i, j = x, y, z$. k_B is the Boltzmann constant

and T is the absolute temperature. $< ... >$ denotes an ensemble average over the distribution of noise. $\delta(t)$ is the Dirac delta function. Imposing reflecting boundary conditions in the transverse direction ensures the confinement of the dynamics within the tube, while periodic boundary conditions are enforced along the longitudinal direction. f is a load against the Brownian motor along the x direction. The shape of the tube is described by its radius,

$$\omega(x) = a[\sin(\frac{2\pi x}{L}) + \frac{\Delta}{4}\sin(\frac{4\pi x}{L})] + b, \tag{4}$$

where a is the parameter that controls the slope of the tube, Δ is the asymmetry parameter of the tube shape and L is its periodicity. The radius at the bottleneck is $r_b = b - a(1+\frac{\Delta}{4})$. $F(t)$ is a temporally symmetric unbiased external force and satisfies

$$F(t) = \begin{cases} F_0, & n\tau \leq t < n\tau + \frac{1}{2}\tau; \\ -F_0, & n\tau + \frac{1}{2}\tau < t \leq (n+1)\tau, \end{cases} \tag{5}$$

where τ is the period of the unbiased force and F_0 is its magnitude.

The movement equation of a Brownian particle moving along the axis of the 3D (or 2D) tube can be described by the Fick-Jacobs equation [11, 12, 13, 23, 24] which is derived from the 3D (or 2D) Smoluchowski equation after elimination of y and z coordinates by assuming equilibrium in the orthogonal directions. The complicated boundary conditions of the diffusion equation in irregular channels can be greatly simplified by introducing an entropic potential that accounts for the reduced space accessible for diffusion of the Brownian particle. Reduction of the coordinates may involve the appearance of entropic barriers and an effective diffusion coefficient. When $|\omega'(x)| << 1$, the effective diffusion coefficient reads [11, 12, 13, 23, 24]

$$D(x) = \frac{D_0}{[1+\omega'(x)^2]^\alpha}, \tag{6}$$

where $D_0 = k_B T/\gamma$ and $\alpha = 1/3$, $1/2$ for two and three dimensions, respectively. The prime stands for the derivative with respect to the space variable x.

Consider the effective diffusion coefficient and the entropic barriers, the dynamics of a Brownian particle moving along the axis of the 3D (or 2D) tube can be described by the equation [11, 12, 13]

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}[D(x)\frac{\partial P(x,t)}{\partial x} + \frac{D(x)}{k_B T}\frac{\partial A(x,t)}{\partial x}P(x,t)] = -\frac{\partial j(x,t)}{\partial x}, \tag{7}$$

where a free energy $A(x,t) = E - TS = fx - F(t)x - Tk_B \ln h(x)$ is defined [11]: here $E = fx - F(t)x$ is the energy, $S = k_B \ln h(x)$ is the entropy, $h(x)$ is the dimensionless width

$2\omega(x)/L$ in two dimensions, and the dimensionless transverse cross section $\pi[\omega(x)/L]^2$ of the tube in three dimensions. $j(x,t)$ is the probability current density. $P(x,t)$ is the probability density for the particle at position x and at time t. It satisfies the normalization condition and the periodicity condition

$$\int_0^L P(x,t)dx = 1, \qquad P(x,t) = P(x+L,t). \tag{8}$$

If $F(t)$ changes very slowly with respect to t, namely, its period is longer than any other time scale of the system, there exists a quasistatic state. It is noted that the validity of the Fick-Jacobs equation in the limit $T \to 0$ is questionable [24] and the quasistatic approximate method would also fail. However, our study is focus on the intermediate values of temperature, and thus our method is still valid. In this case, by following the method in [1, 2, 3, 4, 5, 6, 11, 12, 13], we can obtain the current

$$j(F(t)) = \frac{k_B T[1-\exp(-\frac{(F(t-f))L}{k_B T})]}{\int_0^L h(x)\exp(\frac{(F(t)-f)x}{k_B T})dx \int_x^{x+L}[1+\omega'(y)^2]^\alpha h^{-1}(y)\exp(-\frac{(F(t)-f)y}{k_B T})dy}. \tag{9}$$

For the given external force $F(t)$ (Eq. (5)), the average current over a period is obtained,

$$J = \frac{1}{\tau}\int_0^\tau j(F(t))dt = \frac{1}{2}[j(F_0)+j(-F_0)], \tag{10}$$

where $j(F_0)$ is a current induced by a constant force $F(t) = F_0$.

According to the energetics [25], the input energy E_{in} per unit time from the external force to the system is given by [15, 25],

$$E_{in} = \frac{1}{t_j - t_i}\int_{x(t_i)}^{x(t_j)} F(t)dx(t). \tag{11}$$

From Eq. (9), the input energy per unit time is

$$E_{in} = \frac{1}{2}F_0[j(F_0) - j(-F_0)]. \tag{12}$$

In order for the system to do useful work, the load force f is applied in a direction opposite to the direction of current in the system. If the current flows in the same direction as the load, no useful work is done. The average work per unit time done over a period is given by

$$W = \frac{1}{2}f[j(F_0)+j(-F_0)]. \tag{13}$$

Thus, the efficiency η of the system to transform the external fluctuation to useful work is given by [15, 25]

$$\eta = \frac{W}{E_{in}} = \frac{f[j(F_0) + j(-F_0)]}{F_0[j(F_0) - j(-F_0)]}. \tag{14}$$

Because of $\frac{j(-F_0)}{j(F_0)} < 0$, Eq. (14) can be rewritten

$$\eta = \frac{f}{F_0}[1 - \frac{2|\frac{j(-F_0)}{j(F_0)}|}{1 + |\frac{j(-F_0)}{j(F_0)}|}]. \tag{15}$$

Equation (15) shows that the efficiency η depends on $|\frac{j(-F_0)}{j(F_0)}|$. When $|\frac{j(-F_0)}{j(F_0)}| \to 0$, the maximum efficiency of the energy transformation is $\eta_{max} = f/F_0$.

RESULTS AND DISCUSSIONS

Because the results from two and three dimensions are very similar, for the convenience of physical discussion, we now mainly investigated the energetics in three dimensions with $k_B = 1$ and $\gamma = 1$. In order to compare with the conventional energetic ratchet [15], we also investigate the current and efficiency in the presence of asymmetric energy barriers on the quasistatic limit[Fig. 1 (b)].

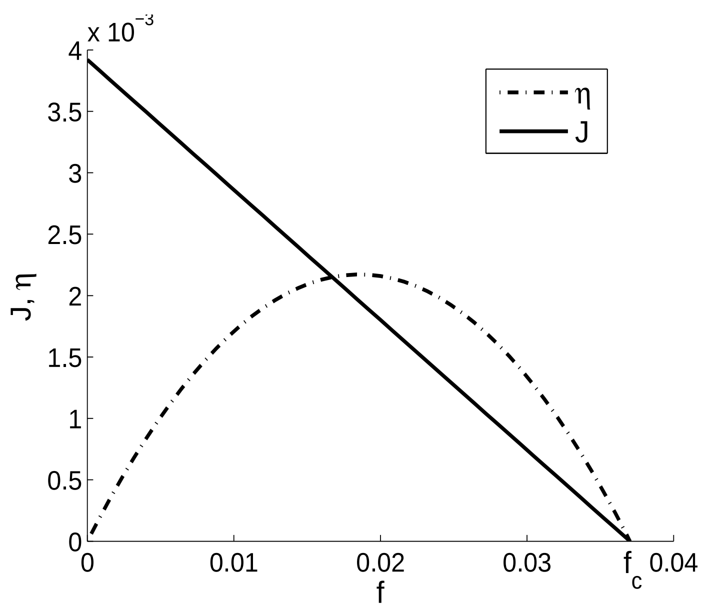

FIG. 2: Efficiency η and current J vs the load f at $a = \frac{1}{2\pi}$, $b = \frac{1.5}{2\pi}$, $L = 2\pi$, $\alpha = 1/2$, $F_0 = 0.5$, $\Delta = 1.0$, and $T = 0.5$. The solid and dash-dotted line denotes J and η, respectively.

In Fig. 2, we plot the efficiency η and current J as a function of the load f in the present system. It is expected that the efficiency exhibits a maximum as a function of the load. It is obvious that the efficiency is zero for the case of zero loading. At the critical value of f_c the current is zero and hence the efficiency also tends to zero. Between $f = 0$ and $f = f_c$ the efficiency exhibits a maximum. Beyond $f = f_c$ the current flows down the load and therefore the definition of efficiency becomes invalid. It is also found that the current is a monotonically decreasing function of the load.

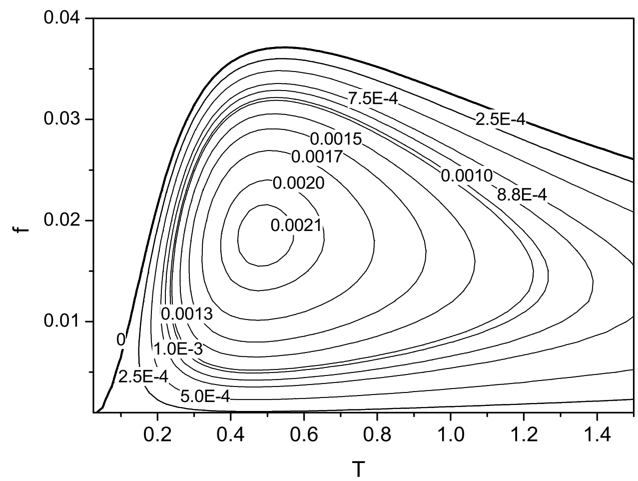

FIG. 3: Efficiency contours on $f - T$ plane at $a = \frac{1}{2\pi}$, $b = \frac{1.5}{2\pi}$, $L = 2\pi$, $\alpha = 1/2$, $F_0 = 0.5$, and $\Delta = 1.0$. The thick solid line indicates $\eta = 0$ contour.

Figure 3 shows the efficiency contours on $f - T$ plane in the present system. The thick solid line indicates $\eta = 0$ contour. When the temperature is low, the maximum load (referring to the critical value of the load f_c in Fig. 2) is small. When the temperature is very high, the maximum load is also small. Therefore there exists a temperature at which the maximum load takes its maximum. The efficiency near the center is high and low far from the center. For a given valid load, the efficiency can be a peaked function of temperature.

Figure 4 shows the current as a function of F_0 for both the present system (a) and the conventional ratchet (b). The current is a peaked function of F_0 for both cases. The current increases with the temperature in present system [Fig. 4(a)]. The current tends to negative at low temperatures ($T = 0.05$) which indicates that the current is dominated by the load

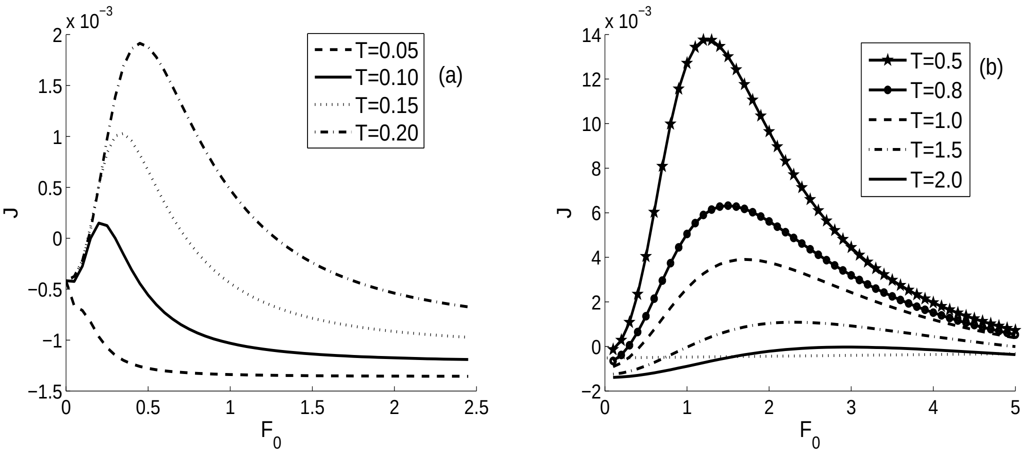

FIG. 4: Current J as a function of F_0 for different values of temperature. (a)Present system at $a = \frac{1}{2\pi}$, $b = \frac{1.5}{2\pi}$, $L = 2\pi$, $\alpha = 1/2$, $\Delta = 1.0$, and $f = 0.01$. (b)The conventional energetic ratchet at $U_0 = 2.0$, $\Delta = 1.0$, $L = 2\pi$, and $f = 0.01$.

f for low temperatures. However, in conventional ratchet the current decreases with the temperature [Fig. 4(b)]. The current goes to negative for high temperatures which shows that the load f dominates at high temperatures ($T = 2.0$).

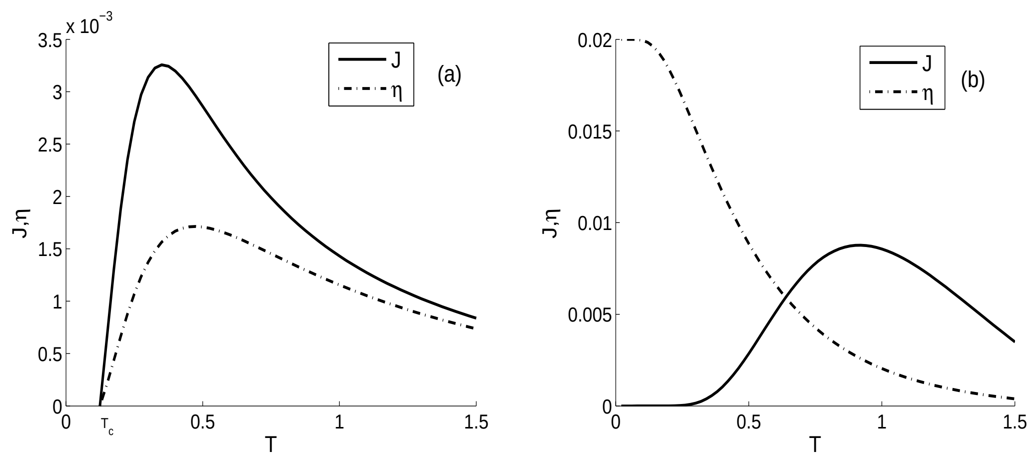

FIG. 5: Efficiency η and current J as a function of temperature T. (a)Present system at $a = \frac{1}{2\pi}$, $b = \frac{1.5}{2\pi}$, $L = 2\pi$, $\alpha = 1/2$, $F_0 = 0.5$, $\Delta = 1.0$, and $f = 0.01$. (b)The conventional energetic ratchet at $U_0 = 2.0$, $\Delta = 1.0$, $L = 2\pi$, $F_0 = 0.5$, and $f = 0.01$.

Figure 5(a) shows the efficiency and current as a function of temperature in present system. The current and efficiency is observed to be bell shaped, which shows the feature

of resonance. When $T \to 0$, the Brownian particle can only move along x axis (1D) and the effect of entropic barriers disappears and the load dominates. Thus, the current is negative. When $T > T_c$, the entropic barriers take effect, the asymmetry of the tube shape can induce a net current [13]. When $T \to \infty$, the effect of the unbiased force disappears and the load dominates, the current becomes negative again. There is an optimized value of T at which the current J takes its maximum. The current in conventional ratchet is similar to that in present system [the solid line in Fig. 5(a) and 5(b)]. However, in the conventional ratchet [15] [the dash-dotted line in Fig. 5(b)] the energetic efficiency of Brownian motors is a monotonically decreasing function of temperature on the quasistatic limit. In that case, thermal noise cannot facilitate energy transformation. Contrary to that work, the efficiency in our system [the dash-dotted line in Fig. 5(a)] is a peaked function of temperature which indicates that thermal noise can facilitate energy conversion. For the case of entropic barriers, even when the current goes to zero at $T = T_c$, local current ($j(F_0)$, $j(-F_0)$) that refers to the current in each semiperiod still remains finite. Thus, there exists finite energy dissipation at $T = T_c$, which shows that the input energy E_{in} still remains finite. Therefore the efficiency is found to zero at $T = T_c$, and takes its maximum at a finite temperature. It is to be mentioned that the temperature corresponding to the maximum efficiency is not the same as the temperature at which the current becomes maximum, which is similar to the case of energetic barriers [4, 17].

In Fig. 6(a) we plot input energy E_{in} and useful work W (scaled up by a factor 200 for convenience of comparison) as a function of temperature. The useful work W has a peak at a finite temperature, because of the behavior of the current during the period τ. The input energy E_{in} is a monotonically decreasing function of temperature. At the limit $T \to 0$, E_{in} tends to its maximum, where all input energy dissipates because in the absence of energetic barriers the unbiased force and the load make finite local current even at the limit $T \to 0$. Therefore the efficiency takes its maximum at a finite temperature. However, in the conventional ratchet [Fig. 6(b)] the input energy E_{in} is a monotonically increasing function of temperature. At the limit $T \to 0$, the current tends to zero and the input energy also goes to zero, which is different from that in the present system.

Figure 7 shows current $j(F_0), j(-F_0)$, and $|\frac{j(-F_0)}{j(F_0)}|$ as a function of temperature for both the present system and the conventional ratchet. The parameters is the same as in Fig. 5. When a constant biased force acts on the motor [Fig. 7(a)], its current decreases monotoni-

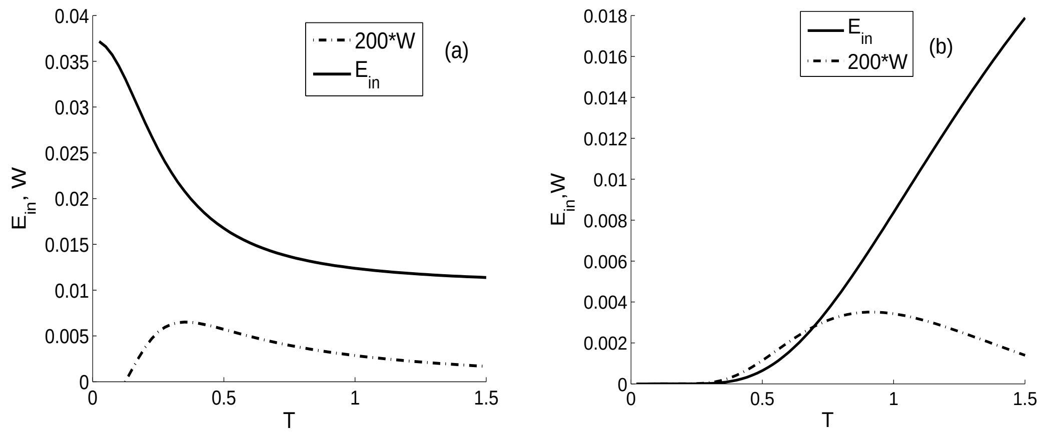

FIG. 6: Useful work W and input energy E_{in} vs temperature (W has been scaled up by a factor of 200 to make it comparable with E_{in}). (a)Present system at $a = \frac{1}{2\pi}$, $b = \frac{1.5}{2\pi}$, $L = 2\pi$, $\alpha = 1/2$, $F_0 = 0.5$, $\Delta = 1.0$, and $f = 0.01$. (b)The conventional energetic ratchet at $U_0 = 2.0$, $\Delta = 1.0$, $L = 2\pi$, $F_0 = 0.5$, and $f = 0.01$.

cally with temperature which is contrary to the case of energetic barriers [Fig. 7(c)] [15, 17]. In the presence of energetic barriers [Fig. 7(c)], the temperature facilitates the activation and thus tends to increase the particle current. However, in the presence of entropic barriers [Fig. 7 (a)], the temperature dictates the strength of the entropic barriers and thus an increasing temperature leads to reduction of the current. Equation (15) shows that the efficiency η depends on $|\frac{j(-F_0)}{j(F_0)}|$. Figure 7 (b) shows that in the presence of entropic barriers the ratio $|\frac{j(-F_0)}{j(F_0)}|$ displays a clear minimum at the same value of temperature which corresponds to a maximum of η in Fig. 5(a). However, in conventional ratchet the ratio $|\frac{j(-F_0)}{j(F_0)}|$ is a monotonically increasing function of temperature [Fig. 7 (d)] and thus the efficiency is a monotonically decreasing function of temperature [Fig. 5(b)]. So the thermal noise cannot facilitate energy transformation in this case.

CONCLUDING REMARKS

In this paper, we study the energetics of a Brownian particle moving along the axis of a three-dimensional asymmetric periodic tube in the presence of a symmetric unbiased force and a load. The movement of the Brownian particle can be described by Fick-Jacobs

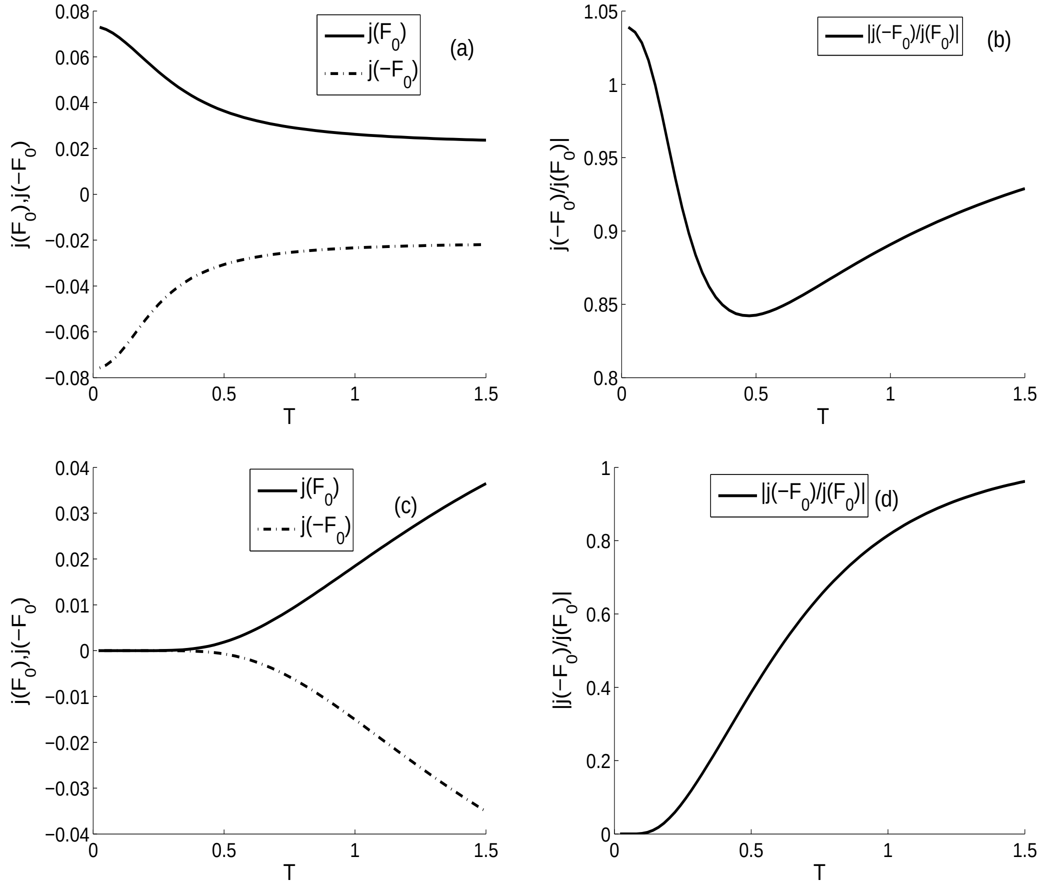

FIG. 7: Plot of currents $j(F_0), j(-F_0)$, and $|\frac{j(-F_0)}{j(F_0)}|$ for both the present system and the conventional ratchet. The parameters is the same as in Fig. 5. (a) $j(F_0)$ and $j(-F_0)$ vs T in present system; (b)$|\frac{j(-F_0)}{j(F_0)}|$ vs T in present system; (c)$j(F_0)$ and $j(-F_0)$ vs T in the conventional energetic ratchet; (d)$|\frac{j(-F_0)}{j(F_0)}|$ vs T in the conventional energetic ratchet.

equation which is derived from 3D (or 2D) Smoluchowski equation after elimination of y and z coordinates. Reduction of coordinates may induce the appearance of entropic barriers and an effective diffusion coefficient. In order to compare with the conventional energetic ratchet on the quasistatic limit, the current and the efficiency are also investigated in the presence of energy barriers. The energetics in the presence of entropic barriers is different from that occurring through energy barriers. It is found that even on the quasistatic limit the efficiency can be a peaked function of temperature, which proves that thermal noise can facilitate energy transformation, contrary to the conventional energetic ratchet [15]. Two factors are essential for the energy transformation activated by thermal noise: first

one is the noise-induced flow, and the second one is the finite dissipation in the absence of thermal noise. For the case of entropic barriers, even when the current goes to zero at $T = T_c$, local current still remains finite. The input energy is a monotonically decreasing function of temperature. Therefore at the limit $T \to 0$, the input energy E_{in} tends to its maximum, where all input energy dissipates. The useful work takes its maximum at a finite temperature. Thus, the efficiency can be a peaked function of temperature. It is to be noted that the condition of maximum current does not correspond to maximum efficiency, which is similar to the case of energy barriers [4, 17].

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